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AG_M AND HM_M INDICES OF LINE GRAPHS OF SUBDIVISION GRAPHS OF SOME MOLECULAR STRUCTURES

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ABSTRACT. Topological indices prove to be a bridge between structural chemistry and mathematics. There are many advances in the studies on topological indices till date. In this paper we define the modified arithmetico-geometrico topological index and modified harmonic mean index and estimate these topological indices for subdivision graphs of certain molecular structures.

1. INTRODUCTION

Topological indices have contributed significantly to the growth of mathematical chemistry and it attracts the attention of chemical and mathematical researchers.Since the initiation of the topic by Gutman and Trinajstic in 1972 [1] various topological indices were defined till date.Several kinds of topological indices, such as Wiener index [5],Arithmetico-geometrico index [3], [4] and Harmonic mean index [2],etc. are all based on vertex-degree of graphs.In this paper we define the modified arithmetico-geometrico topological index and modified harmonic mean index and estimate these toplogical indices for subdivision graphs of certain chemical structures like cyclic hexagonal square chain and nanocone.

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A graph $G = (V, E)$ considered in this paper is simple,finite,undirected graphs with $|V| = p$ vertices and $|E| = q$ edges.For $t \in V(G), N_G(t)$ denotes the set of all neighbours of t in G and $\zeta_G(t)$ denotes the neighbourhood sum of t,defined as $\zeta_G(t) = \sum_{r \in N_G(t)} \delta(r)$ where $\delta(r)$ is the degree of the vertex r.

Definition 1.1. *Modified Arithmetico-geometrico topological index of a non-empty graph G is denoted by $AG_M(G)$ and is defined as*

$$AG_M(G) = \sum_{rs \in E(G)} \frac{\zeta_G(r) + \zeta_G(s)}{2\sqrt{\zeta_G(r)\zeta_G(s)}},$$

where $\zeta_G(r)$ and $\zeta_G(s)$ are the neighbourhood sum of vertices r and s.

Definition 1.2. *Modified Harmonic mean index of a graph G is denoted by $HM_M(G)$ and defined as*

$$HM_M(G) = \sum_{rs \in E(G)} \frac{2\zeta_G(r)\zeta_G(s)}{\zeta_G(r) + \zeta_G(s)},$$

where $\zeta_G(r)$ and $\zeta_G(s)$ are the neighbourhood sum of vertices r and s.

In this paper we consider line graphs of subdivision graphs of cyclic hexagonal square chain and nanocones,which are two molecular structures.For a given graph,subdivision graph can be obtained by inserting a vertex into each of the edges,so that edges get doubled.The line graph of this subdivision graph contain as many vertices as the edges in the subdivion graph and two vertices e and f are incident if and only if they have common end vertex in the subdivision graph.

2. AG_M AND HM_M INDICES OF LINE GRAPH OF SUBDIVISION GRAPH OF CYCLIC HEXAGONAL SQUARE CHAIN $\mathscr{C}_{mn}$

Theorem 2.1. *Let τ be the line graph of the subdivision graph of $\mathscr{C}_{mn}$. Then*

$$AG_M(\tau) \approx 13mn + 9n;$$

$$HM_M(\tau) \approx 95mn + 81n.$$

Proof. The graph of cyclic hexagonal square chain consists of n mutually isomorphic hexagonal chains H_i each containing m hexagons,cyclically augmented by cycle of length 4.$\mathscr{C}_{mn}$ contain $4mn + 2n$ vertices and $5mn + 3n$ edges.The edges can be partitioned into six categories as follows.

$E_1 = \{rs \in E(\tau) | \zeta_\tau(r) = \zeta_\tau(s) = 4\}$

$E_2 = \{rs \in E(\tau) | \zeta_\tau(r) = 4, \zeta_\tau(s) = 5\}$
$E_3 = \{rs \in E(\tau) | \zeta_\tau(r) = 5, \zeta_\tau(s) = 8\}$
$E_4 = \{rs \in E(\tau) | \zeta_\tau(r) = 8 = \zeta_\tau(s)\}$
$E_5 = \{rs \in E(\tau) | \zeta_\tau(r) = 8, \zeta_\tau(s) = 9\}$
$E_6 = \{rs \in E(\tau) | \zeta_\tau(r) = 9 = \zeta_\tau(s)\}$,

where E_1 has mn edges, E_2 has $2mn$ edges, E_3 has $2mn$ edges, E_4 has $mn - n$ edges, E_5 has $2mn + 2n$ edges and E_6 has $5mn + 8n$ edges. Now,

$$\begin{aligned}
AG_M(\tau) &= \sum_{rs \in E(\tau)} \frac{\zeta_\tau(r) + \zeta_\tau(s)}{2\sqrt{\zeta_\tau(r)\zeta_\tau(s)}} \\
&= \sum_{i=1}^{6} \sum_{E_i} \frac{\zeta_\tau(r) + \zeta_\tau(s)}{2\sqrt{\zeta_\tau(r)\zeta_\tau(s)}} \\
&= mn \left[\frac{4+4}{2\sqrt{4.4}}\right] + 2mn \left[\frac{4+5}{2\sqrt{4.5}}\right] + 2mn \left[\frac{5+8}{2\sqrt{5.8}}\right] + (mn - n) \left[\frac{8+8}{2\sqrt{8.8}}\right] \\
&\quad + (2mn + 2n) \left[\frac{8+9}{2\sqrt{8.9}}\right] + (5mn + 8n) \left[\frac{9+9}{2\sqrt{9.9}}\right] \\
&= 13.0714mn + 9.0035n \\
&\approx 13mn + 9n
\end{aligned}$$

$$\begin{aligned}
HM_M(\tau) &= \sum_{rs \in E(\tau)} \frac{2\zeta_\tau(r)\zeta_\tau(s)}{\zeta_\tau(r) + \zeta_\tau(s)} \\
&= \sum_{i=1}^{6} \sum_{E_i} \frac{2\zeta_\tau(r)\zeta_\tau(s)}{\zeta_\tau(r) + \zeta_\tau(s)} \\
&= mn \left[\frac{2.4.4}{4+4}\right] + 2mn \left[\frac{2.4.5}{4+5}\right] + 2mn \left[\frac{2.5.8}{5+8}\right] \\
&\quad + (mn - n) \left[\frac{2.8.8}{8+8}\right] + (2mn + 2n) \left[\frac{2.8.9}{8+9}\right] + (5mn + 8n) \left[\frac{2.9.9}{9+9}\right] \\
&= 95.1378mn + 80.9412n \\
&\approx 95mn + 81n
\end{aligned}$$

□

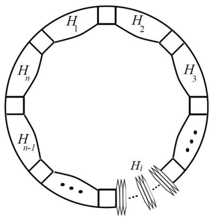

FIGURE 1. $\mathscr{C}_{mn}$

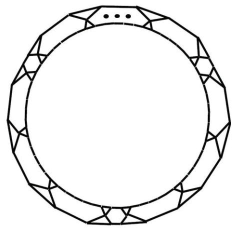

FIGURE 2. Line graph of subdivision graph of $\mathscr{C}_{mn}$

3. AG_M AND HM_M INDICES OF LINE GRAPH OF SUBDIVISION GRAPH OF NANOCONES

Theorem 3.1. *Let τ_1 be the line graph of Subdivision graph of $CNC_k[n]$. Then*

$$AG_M(\tau_1) \approx 2k + 6kn + \frac{9kn^2 + n}{2},$$
$$HM_M(\tau_1) \approx 8k + 42kn + 9\left[\frac{9kn^2 + n}{2}\right].$$

Proof. The graph of nanocones $CNC_k[n]$ consists of a cycle of length k at its centre and n levels of hexagons are placed at the conical exterior around the central cycle. The graph of nanocones and its Line graph of Subdivision graph are shown below.

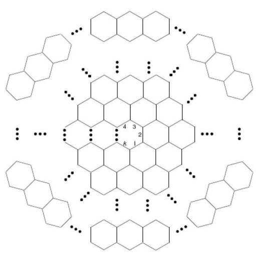

FIGURE 3. Nanocone, $CNC_k[n]$

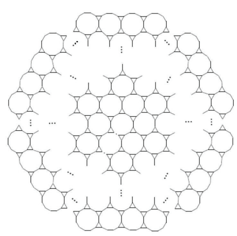

FIGURE 4. Line graph of subdivision graph of $CNC_k[n]$

The edge set $E\tau_1$ can be partitioned into seven categories, such that $E\tau_1 = \sum_{i=1}^{7} E_i$ as follows

$$E_1 = \{rs \in E(\tau) | \zeta_\tau(r) = \zeta_\tau(s) = 4\}$$
$$E_2 = \{rs \in E(\tau) | \zeta_\tau(r) = 4, \zeta_\tau(s) = 5\}$$
$$E_3 = \{rs \in E(\tau) | \zeta_\tau(r) = 5, \zeta_\tau(s) = 5\}$$
$$E_4 = \{rs \in E(\tau) | \zeta_\tau(r) = 5, \zeta_\tau(s) = 8\}$$
$$E_5 = \{rs \in E(\tau) | \zeta_\tau(r) = 8 = \zeta_\tau(s)\}$$
$$E_6 = \{rs \in E(\tau) | \zeta_\tau(r) = 8, \zeta_\tau(s) = 9\}$$
$$E_7 = \{rs \in E(\tau) | \zeta_\tau(r) = 9 = \zeta_\tau(s)\}$$

E_1 has k edges, E_2 has $2k$ edges, E_3 has $k(n-1)$ edges, E_4 has $2kn$ edges, E_5 has kn edges and E_6 has $2kn$ edges and E_7 has $\frac{9kn^2+n}{2}$. Hence,

$$\begin{aligned}
HM_M(\tau_1) &= \sum_{rs \in E(\tau_1)} \frac{2\zeta_\tau(r)\zeta_\tau(s)}{\zeta_\tau(r)+\zeta_\tau(s)} = \sum_{i=1}^{7}\sum_{E_i} \frac{2\zeta_\tau(r)\zeta_\tau(s)}{\zeta_\tau(r)+\zeta_\tau(s)} \\
&= k\left[\frac{2.4.4}{4+4}\right] + 2k\left[\frac{2.4.5}{4+5}\right] + k(n-1)\left[\frac{2.5.5}{5+5}\right] \\
&\quad + 2kn\left[\frac{2.5.8}{5+8}\right] + kn\left[\frac{2.8.8}{8+8}\right] + 2kn\left[\frac{2.8.9}{8+9}\right] + \frac{9kn^2+n}{2}\left[\frac{2.9.9}{9+9}\right] \\
&= 7.8889k + 42.2489kn + 9\left[\frac{9kn^2+n}{2}\right] \\
&\approx 8k + 42kn + 9\left[\frac{9kn^2+n}{2}\right]
\end{aligned}$$

$$\begin{aligned}
AG_M(\tau_1) &= \sum_{rs \in E(\tau_1)} \frac{\zeta_\tau(r)+\zeta_\tau(s)}{2\sqrt{\zeta_\tau(r)\zeta_\tau(s)}} = \sum_{i=1}^{7}\sum_{E_i} \frac{\zeta_\tau(r)+\zeta_\tau(s)}{2\sqrt{\zeta_\tau(r)\zeta_\tau(s)}} \\
&= k\left[\frac{4+4}{2\sqrt{4.4}}\right] + 2k\left[\frac{4+5}{2\sqrt{4.5}}\right] + k(n-1)\left[\frac{5+5}{2\sqrt{5.5}}\right] + 2kn\left[\frac{5+8}{2\sqrt{5.8}}\right] \\
&\quad + kn\left[\frac{8+8}{2\sqrt{8.8}}\right] + 2kn\left[\frac{8+9}{2\sqrt{8.9}}\right] + \frac{9kn^2+n}{2}\left[\frac{9+9}{2\sqrt{9.9}}\right] \\
&= 2.01246k + 6.05895kn + \frac{9kn^2+n}{2} \approx 2k + 6kn + \frac{9kn^2+n}{2}
\end{aligned}$$

□

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